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DETERMINATION OF THE EXCITED STATE DENSITY FOR AN OPTICALLY THICK RESONANCE LINE

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Abstract

The transverse profile of the monochromatic radiance of an optically thick resonance line from a cylindrical discharge is inverted exactly to give the radial distribution of radiating atoms. In contrast to the Abel transform, this result is valid for all optical depths.

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1 Analysis

Determination of the source function for a radiating cylindrical plasma from the transverse profile of the monochromatic radiance of the discharge is a diagnostic technique with a long history.[1,2] If the discharge is optically thin, then the Abel transform[3] applied to the profile of the radiance yields the radial dependence of the source function. For the optically thick case, various approximation schemes[4,5] have been proposed to invert the profile of the radiance. We present a solution to this problem for a resonance line in a weakly ionized plasma that is exact for arbitrary optical depth. A typical application of this result is an explicit expression for the radial dependence of the density of Hg atoms in the $^3P_1$ excited state in a Hg-Ar discharge from the transverse profile of the radiance of the 253.7 nm line.

For a resonance line in the weakly ionized plasma of a discharge, we can assume that the density of atoms in the ground state is constant throughout the cross section of the discharge. Therefore, the absorption coefficient Λ at a fixed wave length in the line is also a constant. Under these conditions, the monochromatic radiance from a small area of the cylinder which is offset from the axis by a distance pR, where R is the radius of the cylinder (see Fig. 1) and is given by

$$I = \Lambda \int_{-\xi_o}^{\xi_o} d\xi \; e^{-\Lambda(\xi_o - \xi)} \; f(p^2 + \xi^2) \; , \tag{1}$$

with $\xi_o = (1 - p^2)^{1/2}$ and Λ is equal to the dimensionless optical depth. While Λ is normally taken to be real, our solution given below applies equally well to situations with a complex Λ. In terms of the angle θ between the direction of the radiation and the normal to the surface of the cylinder, we have $p = \sin\theta$ and $\xi_o = \cos\theta$. In Eq. (1), f is the radial distribution of excited atoms radiating at the observed wave length. Equation (1) is a useful diagnostic if it can be inverted to yield f for an experimentally given I.

Equation (1) can be cast in a more convenient form by defining

$$q = p^2 \ , \ x = p^2 + \xi^2 \ , \ F(\Lambda \ , \ q) = e^{\Lambda \xi_o} I/\Lambda \ . \tag{2}$$

We then have

$$F(\Lambda \ , \ q) = \int_q^1 dx \ (x - q)^{-1/2} \cosh[\Lambda(x - q)^{1/2}] \ f(x) \ . \tag{3}$$

For an optically thin line, $\Lambda \to 0$, the hyperbolic cosine in Eq. (3) is approximated by one and the equation becomes a special case of the Abel[3] equation the solution of which is given by

$$f(x) = - \frac{1}{\pi} \int_x^1 dq \ (q - x)^{-1/2} \frac{\partial F(0,q)}{\partial q} \ . \tag{4}$$

This result has been widely used to obtain the radial distribution of excited states that give rise to optically thin lines. The distribution of atoms giving rise to thick lines can be inferred from a distribution producing a thin line by making the assumption of local thermodynamic equilibrium (LTE) in which the radial dependence of each distribution is through a Boltzman factor containing a common radially varying temperature. However, the assumption of LTE is not valid for typical discharge conditions in which the atoms are radiating energy received from electrons whose temperature is about 12,000 K to an environment at room temperature. Alternatively, various approximation schemes have been developed for inverting Eq. (3) for non-zero Λ (see Refs. 4 and 5 for examples). We have inverted Eq. (3) for arbitrary values of Λ with the result

$$f(x) = -\frac{1}{\pi}\int_x^1 dq\ (q - x)^{-1/2}\cos[\Lambda\ (q - x)^{1/2}]\ \frac{\partial F(\Lambda,q)}{\partial q}\ . \tag{5}$$

This solution includes the Abel solution (4) as a special case for $\Lambda \rightarrow 0$. The details for this solution are presented below

The derivation of Eq. (5) proceeds in three steps. We first develop another integral equation for f from Eq. (3). We then solve this integral equation as a power series in powers of Λ^2. Finally, we sum the series to obtain Eq. (5).

In order to obtain an integral equation for f, we first expand F in powers of Λ^2

$$F(\Lambda\ ,\ q) = \sum_{n=0}^{\infty}\ [\Lambda^{2n}/(2n)!]\ F_n(q)\ , \tag{6}$$

where

$$F_n(q) = \int_q^1 dx\ (x - q)^{n-1/2}\ f(x)\ . \tag{7}$$

Following a generalization of the steps[3] leading to Eq. (4) we consider

$$\phi_n(z) = \int_z^1 dx\ (x - z)^n\ f(x) \tag{8}$$

$$= [2^n\ n!/\pi(2n - 1)!!] \int_z^1 dx \int_z^x dy\ (y - z)^{-1/2}\ (x - y)^{n-1/2}\ f(x)\ , \tag{9}$$

where we have used†

$$\int_z^x dy\ (y - z)^{-1/2}\ (x - y)^{n-1/2} = [\pi(2n - 1)!!/2^n n!]\ (x - z)^n\ . \tag{10}$$

Using Dirichlet's formula[3] to reverse the order of integration in Eq. (8) and the definition of F_n (7), we have

$$\phi_n(z) = [2^n n!/\pi(2n - 1)!!] \int_z^1 dq\ (q - z)^{-1/2}\ F_n(q)\ . \tag{11}$$

We now form the function

$$\sum_{n=0}^{\infty} [\Lambda^{2n}/(2n)!]\ [(2n - 1)!!/2^n n!]\ \ \phi_n\ (z)$$

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†This integral can be evaluated by changing the integration variable to $y' = (y - z)/(x - z)$ and noting that the resultant integral is a beta function which can be evaluated in terms of gamma functions (see Ref.6).

$$= 1/\pi \int_z^1 dq\ (q - z)^{-1/2}\ F(\Lambda\ ,\ q) \tag{12}$$

$$= \int_z^1 dx\ G\left[\frac{\Lambda^2}{4}\ (x - z)\right]\ f(x)\ , \tag{13}$$

where

$$G(y) = \sum_{n=0}^{\infty} [y^n/(n!)^2] = I_0\ (2y^{1/2}) \tag{14}$$

is a Bessel function. We have used Eqs. (6) and (11) to first obtain Eq. (12) and then Eq. (8) to obtain Eq. (13). We now integrate the rhs of Eq. (12) by parts, using $F(\Lambda, 1) = 0$ to drop the surface terms, and equate the result with Eq. (13). This equation is then differentiated with respect to z, using $G(0) = 1$, to obtain the integral equation for f

$$f(z) + \frac{\Lambda^2}{4} \int_z^1 dx\ G'\left[\frac{\Lambda^2}{4}\ (x - z)\right]\ f(x) = -\ (1/\pi) \int_z^1 dq\ (q - z)^{-1/2}\ \frac{\partial F(\Lambda\ ,\ q)}{\partial q}, \tag{15}$$

where

$$G'(y) = \frac{dG(y)}{dy} = \sum_{n=o}^{\infty} [y^n/n!(n + 1)!] = y^{-1/2}\ I_1\ (2y^{1/2}) \tag{16}$$

is proportional to another Bessel function. Equation (15) is the desired integral equation which is to be solved for f. It clearly yields the Abel solution (4) in the limit $\Lambda \to o$.

In practice F and hence the rhs of Eq. (15) are a functions given by experimental observation, while f is determined by inverting Eq. (15). We do this by making a formal expansion of f in powers of $\Lambda^2/4$ which appears on the lhs of Eq. (15) for a fixed and given function on the rhs, i.e.,

$$f(z) = \sum_{n=o}^{\infty} (\Lambda/2)^{2n} f_n(z) , \tag{17}$$

where, from Eqs. (15) and (16), the f_n satisfy the recursion relations

$$f_n(z) = - \sum_{m=0}^{n-1} \int_z^1 dx \frac{(x - z)^{n-m-1}}{(n-m-1)!\ (n-m)!} f_m(x) , \quad n > 0 , \tag{18}$$

and

$$f_o(z) = - (1/\pi) \int_z^1 dq \ (q \quad z)^{-1/2} \partial F(\Lambda , q)/\partial q . \tag{19}$$

Equations (18) and (19) have the solution

$$f_n(z) = - [(-4)^n/\pi(2n)!] \int_z^1 dq \ (q - z)^{n-1/2} \partial F(\Lambda , q)/\partial q . \tag{20}$$

The details of this solution are given in the Appendix. Substitution of this result into Eq. (17) and summing the series yields our principal result given by Eq. (5).

Equation (5) has the unusual property that f on the lhs is independent of Λ and yet there seems to be an explicit Λ-dependence on the rhs. That there is no true Λ-dependence can be shown by substituting Eq. (3) into Eq. (5), expanding in powers of Λ^2, showing that only the term proportional to Λ^0 is different from zero and that this term is the Abel solution Eq. (4). Thus, the higher order terms in the expansion in Eq. (17) compensate for the Λ-dependence in the lowest order term Eq. (19).

The meaning of our result may be clarified by a simple example. We assume that the radial distribution of excited states is parabolic, proportional to $1 - (r/R)^2$. Then $f(x) = 1 - x$ up to an overall factor. Substitution into Eq. (1) yields

$$I = (4e^{-\Lambda\xi_o}/\Lambda^2)\ [\Lambda\xi_o \cosh \Lambda\xi_o - \sinh\Lambda\xi_o] \tag{21}$$

and, from the definition of F Eq. (2),

$$\partial F(\Lambda\ , q)/\partial q = -\ (2 \sinh\Lambda\xi_o)/\Lambda \tag{22}$$

Substituting into Eq. (5) yields

$$f(x) = (1 - x)\ (2/\pi\bar{\Lambda}) \int_0^1 dy\ y^{-1/2} \cos\bar{\Lambda}y^{1/2} \sinh\bar{\Lambda}\ (1 - y)^{1/2}, \tag{23}$$

where $\bar{\Lambda} = \Lambda(1 - x)^{1/2}$ and we have changed integration variables from q to $y = (q - x)/(1 - x)$. The integral in Eq. (23) can be done by expanding in powers of $\bar{\Lambda}$ and integrating term by term. Only the lowest order term is different from zero with all higher order terms vanishing due to destructive interference from terms coming from the cosine and those from the hyperbolic sine. The lowest order term is proportional to a beta function which can be evaluated in terms of gamma functions and cancels the factor $2/\pi\bar{\Lambda}$. Thus, the output function (23) equals the input function $1 - x$.

The evaluation of f using Eq. (5) from an empirically given F may pose some problems. If we change variables as in the example, we have

$$f(x) = -(1/\pi)\ (1 - x)^{1/2} \int_0^1 dy\ y^{-1/2}\ \cos\bar{\Lambda}y^{1/2}\ \partial F(\Lambda\ ,\ q)/\partial q|_{q\ =\ x\ +\ (1\ -\ x)y}\ . \tag{24}$$

We have first the errors incurred by evaluating $\partial F/\partial q$ from an empirically given F. This problem is common to all applications of the Abel transform. The additional problem is due to the cosine in Eq. (24) whose argument will be large for large Λ and therefore it will oscillate rapidly as a function of y. On the other hand, $-\ \partial F/\partial q$ will be a smooth decreasing function of q as in Eq. (22). These features may provide a basis for the development of efficient numerical methods for evaluating Eq. (24)

An interesting alternative solution to Eq. (3) which does not seem to have a practical application follows from the relation

$$\int_0^{\Lambda} \Lambda' d\Lambda'\ G\left[\frac{\Lambda'^2}{4}\ (x - z)\right] = \frac{\Lambda^2}{2}\ G'\left[\frac{\Lambda^2}{4}\ (x - z)\right]\ . \tag{25}$$

This expression follows from the power series expansions given in Eqs. (14) and (16). Thus, the second term on the lhs of Eq. (15) can be written as

$$\frac{\Lambda^2}{4} \int_z^1 dx\ G'\left[\frac{\Lambda^2}{4}\ (x - z)\right]\ f(x) = 1/2 \int_z^1 dx \int_0^\Lambda \Lambda' d\Lambda'\ G\left[\frac{\Lambda'^2}{4}\ (x - z)\right]\ f(x)$$

$$= 1/2 \int_0^\Lambda \Lambda' d\Lambda'\ \frac{1}{\pi} \int_z^1 dq\ (q - z)^{-1/2}\ F(\Lambda', q) \ ,$$

where we have interchanged the order of intergration and used Eqs. (12) an (13) to perform the x-integration. This result leads to the solution

$$f(x) = -(1/\pi) \int_x^1 dq\ (q - x)^{-1/2}\ [\partial F(\Lambda, q)/\partial q + 1/2 \int_o^\Lambda \Lambda' d\Lambda'\ F(\Lambda', q)] \ . \tag{26}$$

The first term in the square brackets reproduces the Abel solution, for $\Lambda \to 0$, and the second term compensates for the Λ-dependence of the first for $\Lambda > 0$. This cancelation can be readily verified in the example given above. This solution is not practical because one must know F for $\Lambda \to 0$ in order to evaluate the Λ' integral in Eq. (26). One therefore has the information needed to use the Abel solution.

The use of Eq. (5) enables the experimenter to choose a point on a resonance line on the basis of intensity rather than optical depth. This advantage should greatly facilitate the use of transverse profiles of such lines as discharge tube diagnostics.

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APPENDIX

In this appendix, we verify that Eq. (20) is the solution of the coupled system of integral equations given by Eqs. (18) and (19).

We first note that, for n=0, f_0 given by Eq. (20) satisfies Eq. (19). For $n > 0$, we substitute f_m given by Eq. (20) into the rhs of Eq. (18) and obtain

$$f_n(z) = \frac{1}{\pi} \sum_{m=0}^{n-1} \frac{(-4)^m}{(n-m-1)!(n-m)!(2m)!} \int_z^1 dx \int_x^1 dq \ (x - z)^{n-m-1} \ (q - x)^{m-1/2} \ F'(q) \ , \tag{A.1}$$

where we have defined $F'(q) = \partial F(\Lambda,q)/\partial q$. The integral in the m^{th} term of this sum can be manipulated as follows:

$$\int_z^1 dx \int_x^1 dq \ (x - z)^{n-m-1} \ (q - x)^{m-1/2} \ F'(q)$$

$$= \int_z^1 dq \int_z^q dx \ (x - z)^{n-m-1} \ (q - x)^{m-1/2} \ F'(q) \tag{A.2}$$

$$= \int_z^1 dq \ (q - z)^{n-1/2} \left[\int_0^1 dy \ (1 - y)^{n-m-1} \ y^{m-1/2}\right] F'(q) \ . \tag{A.3}$$

Equation (A.2) follows from Dirichlet's formulae[3] and Eq. (A.3) from a change of integration variables from x to $y = (q - x)/(q - z)$. The y-integral in Eq. (A.3) is a beta function[6] given by

$$B(m + 1/2, n - m) = (n - m - 1)! \ \Gamma(m + 1/2)/\Gamma(n + 1/2).$$

Thus, Eq. (A.1) can be written as

$$f_n(z) = \frac{1}{\pi} \sum_{m=0}^{n-1} \frac{(-4)^m \, \Gamma(m + 1/2)}{(n - m)!(2m)!\Gamma(n + 1/2)} \int_z^1 dq \, (q - z)^{n-1/2} \, F'(q). \tag{A.4}$$

The sum over m in Eq. (A.4) can be evaluated as follows:

$$\sum_{m=0}^{n-1} \frac{(-4)^m \, \Gamma(m + 1/2)}{(n - m)!(2m)! \, \Gamma(n + 1/2)} = \frac{4^n}{(2n)!} \sum_{m=0}^{n-1} \frac{(-)^m \, n!}{m!(n - m)!} \tag{A.5}$$

$$= -(-4)^n/(2n)! \; . \tag{A.6}$$

Equation (A.5) follows from the substitution of the expression

$$\Gamma(m + 1/2) = (2m)! \; \Gamma(1/2)/4^m m!$$

and a similar one for $\Gamma(n + 1/2)$. Equation (A.6) follows from the recognition that the sum on m on the rhs of Eq. (A.5) is the binomial expansion of

$$(1 - s)^n - (-s)^n \; , \text{ with } s \to 1 \; ,$$

and $n > 0$.

Substitution of Eq. (A.6) into Eq. (A.4) yields Eq. (20) and the solution is verified for all n.

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Fig. 1. Cross section of a cylindrical discharge of radius R. The radiance I at a radial offset pR comes from radiating atoms located on the chord extending from $-\xi_o$ R to ξ_o R, where $\xi_o = (1 - p^2)^{1/2}$. The angle between the normal to the surface and the direction of I is θ with $p = \sin\theta$ and $\xi_o = \cos\theta$.

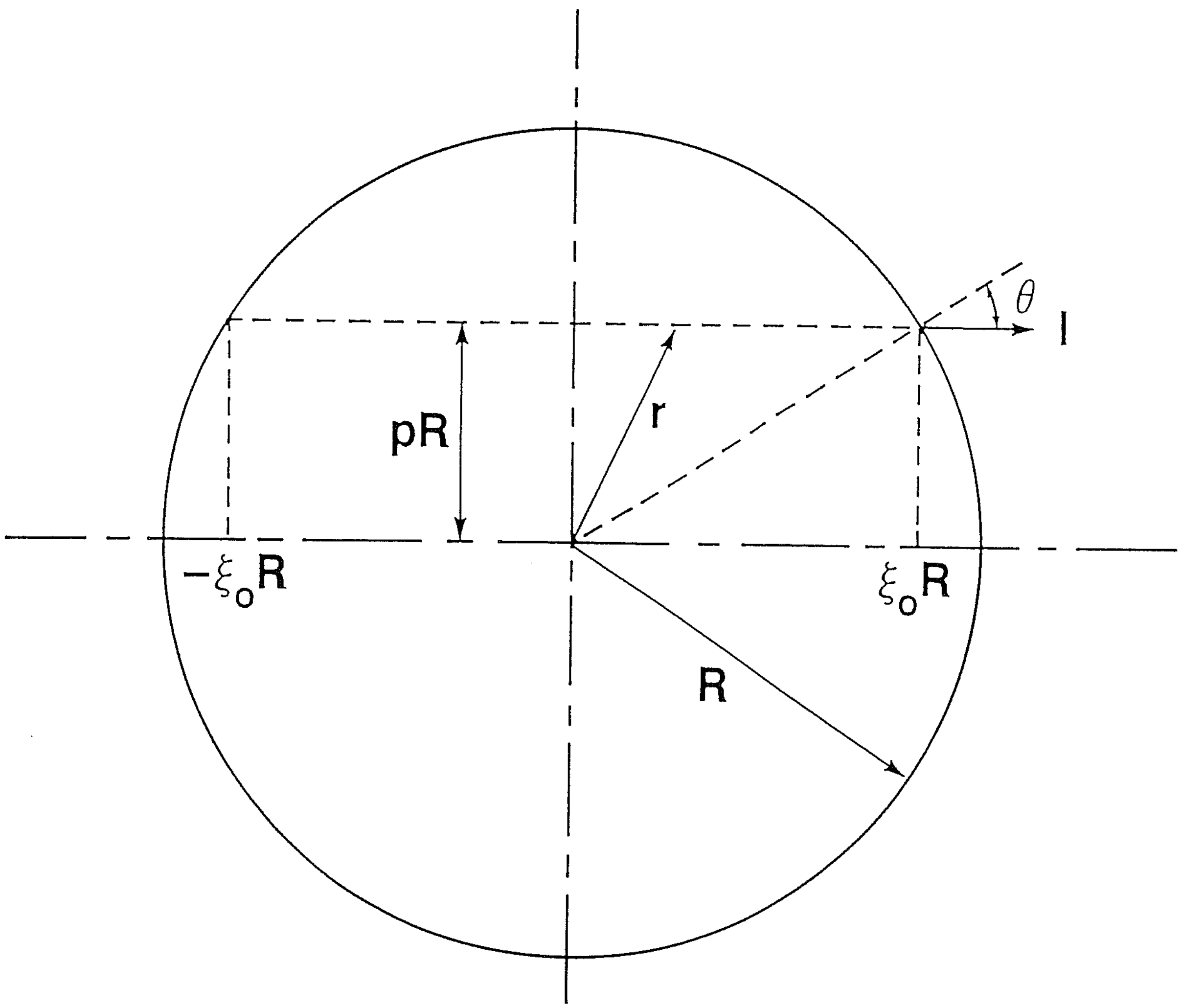

Table 1. Transverse profile of the 253.7 nm resonance line of a Hg-Ar discharge compared with that given by three choices for the radial distribution of $^3P_1$ mercury atoms. The distribution are given by Eq. (23). The experimental data was taken at 45° from an 1 1/2 inch diameter tube filled with 3 torr Ar. The theoretical fits used an optical depth of 100 at line center.

	Experiment	Fit		
p		F_1	F_2	F_3
0.000	1.00	1.00	1.00	1.00
0.105	0.98	0.99	0.98	0.98
0.211	0.94	0.96	0.94	0.91
0.316	0.86	0.91	0.86	0.81
0.421	0.76	0.83	0.76	0.68
0.526	0.64	0.74	0.64	0.53
0.632	0.50	0.62	0.50	0.37
0.737	0.36	0.48	0.36	0.22
0.842	0.22	0.32	0.21	0.09
0.947	0.08	0.12	0.07	0.01
1.000	0.00	0.00	0.00	0.00